

Transition from Solitons to Solitary Waves in the Fermi-Pasta-Ulam Lattice

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Abstract

In this paper, we study the smooth transition from solitons to solitary waves in localization, relation between energy and velocity, propagation and scattering property in the Fermi-Pasta-Ulam lattice analytically and numerically. A soliton is a very stable solitary wave that retains its permanent structure after interacting with other solitary waves. A soliton exists when the energy is small, and it becomes a solitary wave when the energy increases to the threshold. The transition could help to understand the distinctly different heat conduction behaviors of the Fermi-Pasta-Ulam lattice at low and high temperature.

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I. INTRODUCTION

The history of solitary waves can be traced back to 1834, when it was first discovered by Russell on the Union Canal in Scotland [1]. Several decades later Korteweg-de Vries equation was provided which explained the phenomenon mathematically [2]. More than a century later, Fermi, Pasta and Ulam (FPU) investigated the fundamental problem of energy equipartition and ergodicity in nonlinear systems and discovered FPU recurrence [3], which has led eventually to the soliton concept [4]. Since then solitary waves have been studied in various different fields of physics like solid-state physics, quantum theory, nonlinear optics, fluid dynamics, biophysics, etc. [5, 6].

Distinguishing between solitons and solitary waves is sometimes of importance such as studies on energy transport. Solitons are localized solutions of integrable equations, and they are very special types of solitary waves which do not alter form and only have a phase shift after collision with other solitons. Solitary waves are associated with nonintegrable equations, and they are deformed and energy exchange may occur when solitary waves interact with one another [7]. In the long wavelength approximation, the FPU- α and FPU- β lattices lead to the KdV and modified KdV equations, respectively, in which the exact soliton solutions exist. The stability of soliton in the FPU lattice at low

energy is demonstrated [8, 9, 10, 11]. At high energy level, it becomes solitary wave, which makes attribution to heat conduction [12, 13] because of the inelastic scattering between each other. Up to now, very little work has been done on the study of changing from solitons to solitary waves in the FPU lattice.

In this work, we focus on the transition from solitons to solitary waves in the FPU lattice. Previously in numerical work solitons are constructed by using analytical soliton solution directly [14] or starting with a special initial condition [4]. Here we obtain solitons in the FPU lattice for the first time with momentum excitation, which is the widely used method to excite solitary waves [12, 13, 15, 16, 17]. Soliton transforms to solitary wave when energy increases larger than the threshold. Solitons and solitary waves are different in relation between energy and velocity, propagation and scattering behavior. Solitons and solitary waves maintain shape and energy when travelling; kinetic and potential energy remain unchanged for solitons while they are varying periodically for solitary waves. The scattering of solitons is elastic. When two solitary waves collide with each other, both of them lose energy or they exchange energy, and extra wave packets are excited. The solitary wave properties become similar to those in the pure anharmonic lattice when energy tends to infinity. Finally the different heat conduction behaviors of the FPU lattice at low and high temperature are discussed with the concept of solitons and solitary waves.

II. ANALYSIS IN THE WEAKLY NONLINEAR LIMIT

We consider the Hamiltonian for the FPU lattice

$$H = \sum_n H_n, H_n = \frac{p_n^2}{2} + V(q_{n+1} - q_n) \quad (1)$$

$$V(q) = \alpha q^2/2 + \beta q^4/4 \quad (2)$$

where p_n denotes the momentum and q_n denotes the displacement from equilibrium position for the n th atom. Dimensionless units are used, such that the masses, the linear and nonlinear force constants, and the lattice constant are all chosen to be unity. The parameters α and β are the harmonic and anharmonic force constant, respectively. Here $\alpha = 1$ and $\beta = 1$ for the FPU lattice throughout the paper.

The equations of motion of the FPU system are

$$\ddot{q}_n = (q_{n+1} - q_n) + (q_{n-1} - q_n) + (q_{n+1} - q_n)^3 + (q_{n-1} - q_n)^3 \quad (3)$$

In the long wavelength limit, the continuum approximation should be applicable. The displacement $q_{n\pm 1}$ of the $(n \pm 1)$ th lattice is expanded as

$$q_{n\pm 1} = q \pm q_x + \frac{1}{2}q_{xx} \pm \frac{1}{6}q_{xxx} + \frac{1}{24}q_{xxxx} + \cdots \quad (4)$$

where $q(x, t) = q_n(t)$, and $x = n$. Substituting Eq. (4) into Eq. (3) and neglecting higher order terms, we obtain the continuous counterparts of Eq. (3):

$$q_{tt} = (1 + 3q_x^2) q_{xx} + \frac{1}{12} q_{xxxx} \quad (5)$$

We shall be interested in right-going waves, and introduce the new slow variables

$$\xi = 2\varepsilon(x - t), \tau = \varepsilon^3 t \quad (6)$$

and define

$$q(x, t) = \varphi(\xi, \tau) \quad (7)$$

where ε is a formal small parameter. Substituting Eq. (6) and (7) into Eq. (5) and keeping terms in the order of ε^4 , we obtain the following evolution equation for the function $\psi = \partial\varphi/\partial\xi$:

$$\psi_\tau + \frac{3}{2} \psi^2 \psi_\xi + \frac{1}{24} \psi_{\xi\xi\xi} = 0 \quad (8)$$

which is the well known modified Korteweg-de Vries equation. Eq. (8) is derived from the FPU chain [18, 19] and it results in the soliton solutions [14, 20, 21]:

$$q_n = \varphi = -\sqrt{2/3} \arctan\{e^{A\sqrt{6}[n-t-(A/2)^2 t]}\} + c \quad (9)$$

$$p_n = \dot{q}_n = A \left[1 + (A/2)^2 \right] \sec h \{ A\sqrt{6} [n - t - (A/2)^2 t] \} \quad (10)$$

where c is constant. Eq. (9) and (10) are valid if the higher derivatives are neglected. It can be achieved if the following is fulfilled.

$$6A^2 \ll 1 \quad (11)$$

The solutions for q_n and p_n are kink and bell shaped soliton respectively and the soliton velocity is achieved:

$$v = 1 + (A/2)^2 \quad (12)$$

The soliton energy is

$$E = \sum_n \frac{p_n^2}{2} + \sum_n [(q_{n+1} - q_n)^2/2 + (q_{n+1} - q_n)^4/4] \quad (13)$$

The first term of Eq. (13) denotes kinetic energy of soliton and the second term is potential energy. In the long wavelength limit, potential energy is very close to kinetic energy for soliton at low energy, so soliton energy can be expressed as follow:

$$E = 2 \sum_n \frac{p_n^2}{2} \quad (14)$$

Since soliton energy is unchanged as soliton propagates, substituting Eq. (10) at the time $t = 0$ we obtain

$$E = \sum_n \{A [1 + (A/2)^2] \operatorname{sech}(A\sqrt{6}n)\}^2 \quad (15)$$

Replacing the sum by an integral in Eq. (15) due to continuum approximation and using Eq. (11), we finally arrive to

$$E = \frac{2}{\sqrt{6}}A \quad (16)$$

Then we can get the relation between soliton energy and velocity from Eq. (12) and (16) in the case of soliton energy $E \ll \frac{1}{3}$:

$$v = 1 + \frac{3}{8}E^2 \quad (17)$$

So soliton velocity is close to acoustic velocity due to the small energy.

III. HARMONIC LIMIT AND ANHARMONIC LIMIT

We obtain the harmonic lattice in the absence of the quartic term, i.e., $\alpha = 1$ and $\beta = 0$ for Eq. (1) and (2). The system is integrable and can be analytically solved. Here acoustic velocity is 1.

It is the pure anharmonic lattice with $\alpha = 0$ and $\beta = 1$. In this case the excitation, propagation and interaction of solitary waves have been studied in Refs. 13,15, 22, 23. The system has an excellent scaling property, from which we can obtain the relation between energy E and velocity v of a solitary wave:

$$v = aE^{1/4} \quad (18)$$

$a = 0.68198$ from numerical simulations [13].

IV. TRANSITION FROM SOLITONS TO SOLITARY WAVES IN THE FPU LATTICE

Solitary waves can be excited by momentum kicks on the lattice. We apply a kick p_1 on the first lattice at $t = 0$ for static system under the free boundary condition. In Fig. 1 we plot p_i versus i after a short time ($t = 500$) for three kinds of lattices: the harmonic chain at $p_1 = 0.7$ (a), the pure anharmonic chain at $p_1 = 0.7$ (b), the FPU chain at $p_1 = 1.5$ (c) and the FPU chain at $p_1 = 0.7$ (d). In the harmonic chain the amplitude of the wave profile decreases while the width increases with time continuously. In the pure anharmonic chain a solitary wave is excited accompanied by the tail, which is made of several small solitary waves shown in the inset of Fig. 1 (b) [13]. In the FPU chain, at first the wave front is connect with the other low amplitude excitations. If the imparted kick is large enough, after a certain short time, the wave front separates from the tail, because it moves faster. It propagates forward and becomes a solitary wave, just like that in Fig. 1 (c). If the kick is small, the excited wave packet looks like that in the harmonic chain in a short time (Fig. 1 (d)). But actually It will

show the essential difference after a long time. Consider the lattice which is so long that the wave packet won't reach the other end of the lattice in the long observing time. As the first wave pulse travels, its width becomes wider and its peak becomes lower, as shown in Fig. 1 (e) at the time of $t = 10^4$, still like that in the harmonic chain. The speed of the first pulse is calculated and it is a little larger than the acoustic velocity of 1, and so it is not a linear wave. The first pulse travels a little faster than the second pulse, so as long as time is long enough, the first pulse will separate from the second one. Fig. 1 (f) displays the separation of the first pulse from the others at $t = 2 \times 10^5$, and from then on its shape and energy do not change any more, and it becomes a solitary wave. We show this solitary wave in the momentum space and configuration space in Fig. 2. The velocity v and energy E of the solitary wave are calculated numerically: $v = 1.000743$, $E = 0.044664$, and v and E satisfy the relation of Eq. (17). Then the solitary wave may be a soliton solution. A can be obtained from Eq. (12) (Eq. (16)) with $v(E)$. Then we fit the solitary wave with Eq. (10) and (9) in Fig. 2. and the excellent fit shows that the solitary wave excited by the small kick $p = 0.7$ is a soliton indeed.

We present the width of solitary waves at different energy in Fig. 3 (a). The energy of solitary wave is determined by the kick strength and can be calculated with Eq. (13), where the sum is computed over the lattices on which the solitary wave is localized. At the energy of $E < 0.1$ the width of solitary wave is relatively wide and exhibits a power-law decay with energy. At $E > 0.1$ the decay of width becomes slower and the localization of the solitary wave becomes strong as energy increases. At $E > 50$ solitary wave is always localized on the 4 lattices, the same as that in the pure anharmonic lattice.

Fig. 3 (b) shows the relation between energy and velocity of solitary waves in the FPU lattice. If the energy $E < 0.1$, the width of solitary wave is large and the continuum approximation is applicable, so the relation is consistent with Eq. (17) [see the inset in Fig. 3 (b)] and the solitary wave is a soliton. According to Eq. (17), soliton velocity is only a little larger than the acoustic velocity because its energy is so small. If $E > 0.1$, the solitary wave is localized on a few lattices and the long wavelength limit is not satisfied. This leads the deviation from the fitted curve of Eq. (17). So with the increase of energy, the nonlinear part in the interaction potential of Eq. (2) becomes more and more obvious and soliton turns into solitary wave. If $E > 50$, velocity increases with energy as a power-law function, asymptotic to $v = aE^{1/4}$ of Eq. (18) in the pure anharmonic lattice. In this case, the linear part in Eq. (2) is negligible while the nonlinear part is significant, and the property of solitary wave becomes similar to that in the pure anharmonic lattice.

In the following we discuss solitary wave scattering dynamics. Scattering property is an important key to determine whether it is a soliton or a solitary wave. Soliton scattering is elastic while solitary wave scattering is inelastic. Fig. 4 show the process of head-on collision of a pair of solitary wave a and b . The energy of a is one half of that of b , i.e., $E_a/E_b = 1/2$. Before collision each solitary wave maintains shape and energy, as shown in Fig. 4 (a), (c), (e) and (g). After collision the two solitary waves pass through each other,

denoted as a' and b' , and the scattering behaviors are significant different in the following four cases. In Fig. 4 (b), the two solitary waves a and b with $E_a = 0.01$ and $E_b = 0.02$ do not change their shapes and energy and it is an elastic scattering. So a and b are solitons. In Fig 4 (d), solitary wave a with $E_a = 0.05$ is unchanged, i.e., a' is the same as a , while solitary wave b with $E_b = 0.1$ is scattered to solitary wave b' with a tapered tail. The energy of solitary wave b decreases and $E_b = E_{b'} + E_{b't}$, here $E_{b't}$ is the energy of the tail of b' . In Fig 4 (f), both solitary wave a and b with $E_a = 0.1$ and $E_b = 0.2$ are scattered. They are scattered to a' and b' with tapered tails respectively. The energy of a and b decrease. $E_a = E_{a'} + E_{a't}$ and $E_b = E_{b'} + E_{b't}$, $E_{a't}$ is the energy of the tail of a' . In Fig 4 (h), the scattering behavior of solitary waves with $E_a = 0.3$ and $E_b = 0.6$ is quite different from that in Fig 4 (f). Energy exchange takes place and the scattering effect is enhanced. The large solitary wave b loses energy and the small one a gains energy, and extra wave packets are excited. So the collision process varies from elastic to inelastic and then the scattering effect becomes stronger with the increase of the energy of solitary wave.

Next we calculate the energy scattering rate of solitary wave to describe the scattering behavior quantitatively. The energy of a solitary wave is the sum of kinetic energy and potential energy. In the FPU lattice the soliton energy is small and its width is wide. Kinetic energy and potential energy don't varies with time while soliton travels, as shown in Fig. 5 (a), where soliton energy is 0.01. So after collision, the scattering result does not change with time delay of the two solitons, labeled as phase δ [see Fig. 5 (b)]. As energy increases, soliton becomes solitary wave. Solitary wave is only localized on a few lattices. So due to the discrete nature of the lattice, during a solitary wave is travelling on the lattice, its total energy is unchanged while its kinetic energy and potential energy vary with time periodically, as presented in Fig. 5 (c), in which solitary wave energy is 0.3. The variation period T is the time that the solitary wave spends on moving the distance of one lattice constant. Here the lattice constant is unity, and then $T = 1/v$. This leads the scattering results also vary with phase δ periodically [13, 23] [see Fig. 5 (d)]. For practical application, statistical properties are more significant than the prompt values. Then we investigate the average energy scattering rates, $\langle E'_a - E_a \rangle / E_a$, $\langle E'_b - E_b \rangle / E_b$, and the average rate of the energy "loss", $\langle \Delta E \rangle / (E_a + E_b)$.

Fig. 6 present the average energy scattering rates and the average rate of the energy "loss" with the increase of energy when E_a/E_b is fixed as 1/2. When the solitary wave energy $E < 0.1$, the scattering rate is zero and the scattering is elastic. The scattering process is similar to that in Fig. 4 (a) and (b). The shapes and energy of the two solitary waves are unchanged. So the solitary wave with energy $E < 0.1$ is a soliton. When $0.1 < E < 0.3$, the energy scattering rates of a and b are both less than 0 and the scattering is inelastic. The scattering process can be shown by Fig. 4 (e) and (f) approximately. Both of the two solitary waves are scattered into smaller ones with tapered tails and there is no energy exchange between them. The scattering effect is quite weak as the scattering rate is around 10^{-3} . Soliton is transformed into solitary wave

with the increase of energy. When $E > 0.3$, the energy scattering rate is more than 0 for the small solitary wave a and is less than 0 for the large solitary wave b , and the scattering is inelastic. The scattering process is like that in Fig. 4 (g) and (h). There is energy exchange between the two solitary waves, i.e., large solitary wave b loses energy and small one a obtains energy on average, and extra wave packets are excited. The stars in Fig. 6 are the scattering results for the pure anharmonic lattice. Any pair of solitary waves with the same ratio E_a/E_b has the same scattering rates due to the scaling property [13]. In the FPU lattice the scattering effect increases with energy and the scattering results approach those in the pure anharmonic lattice when $E \rightarrow \infty$.

V. CONCLUSION AND DISCUSSION

In summary, we explore the transition from solitons to solitary waves in the FPU lattice. Solitons and solitary waves can be excited by momentum kicks. If energy is smaller than 0.1, the excitation is a soliton, which is consistent with analytical results. Solitons maintain shape and energy, and kinetic and potential energy remain unchanged while travelling. The soliton scattering is elastic; solitons do not alter shape and energy after collision with others. If energy is larger than the threshold of 0.1, soliton transforms to solitary wave. When a solitary wave propagates, kinetic energy and potential energy are varying periodically, while total energy does not change. The solitary wave scattering is inelastic; both of solitary waves lose energy, or large solitary wave loses energy and small one gains on average, and extra wave packets are excited. If energy is large enough, the properties of solitary waves tend to those in the pure anharmonic lattice.

The heat conduction behaviors of the FPU lattice are quite different at low and high temperature. The temperature gradient can't be formed like the harmonic lattice at low temperature, while it can be set up at high temperature [12, 24, 25]. We discuss it with the concept of solitons and solitary waves. In molecular dynamics simulations, the temperature at position n is defined as $T_n = \langle p_n^2 \rangle / 2$ and the role of a thermostat can be interpreted as a series of kicks on the ends of the lattice. When the thermostat temperature is low, solitons are excited. The soliton scattering is elastic and there is no energy exchange, and so there is no temperature gradient formed. In the case of high thermostat temperature, solitary waves are obtained. The solitary wave scattering is inelastic and energy exchange takes place, and so temperature gradient is set up.

ACKNOWLEDGMENT

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Figure Captions

FIG. 1 The momentum p_i versus lattice position i . (a) the harmonic chain at $p_1 = 0.7$ and $t = 500$. (b) the pure anharmonic chain at $p_1 = 0.7$ and $t = 500$.

(c) the FPU chain at $p_1 = 1.5$ and $t = 500$. (d), (e) and (f) represent the FPU chain at $p_1 = 0.7$ with $t = 500$, $t = 10^4$ and $t = 2 \times 10^5$, respectively.

FIG. 2 Dots represent the solitary wave in Fig. 1 (f) in the momentum space (a) and configuration space (b). Solid lines in (a) and (b) stand for fitted curves of Eq. (10) and Eq. (9), respectively.

FIG. 3 The width (a) and velocity (b) versus energy of solitary waves in log-log scale (dots). (a) x axis is the energy of solitary wave E and y axis is the number N of lattices where solitary wave is localized. (b) The solid line is a fit of Eq. (17), and the dashed line is a fit of Eq. (18). The inset enlarges the region indicated by the dotted-line rectangle.

FIG. 4 Head-on collision processes of a pair of solitary wave a and b . (a) and (b), $E_a = 0.01$ and $E_b = 0.02$. (c) and (d), $E_a = 0.05$ and $E_b = 0.1$. (e) and (f), $E_a = 0.1$ and $E_b = 0.2$. (g) and (h), $E_a = 0.3$ and $E_b = 0.6$. (a), (c), (e) and (g) are before collision and (b), (d), (f) and (h) are after collision. Insets in (d), (f) and (h) are enlargement of rectangle.

FIG. 5 (a) and (c), kinetic energy (solid line) and potential energy (dot line) versus time. Soliton energy is 0.01 in (a) and solitary wave energy is 0.3 in (c). (b) and (d), the energy of scattered solitary wave a' versus phase δ . (b) is corresponding to the collision process in Fig. 4 (a) and (b), and (d) is for the process in Fig. 4 (g) and (h).

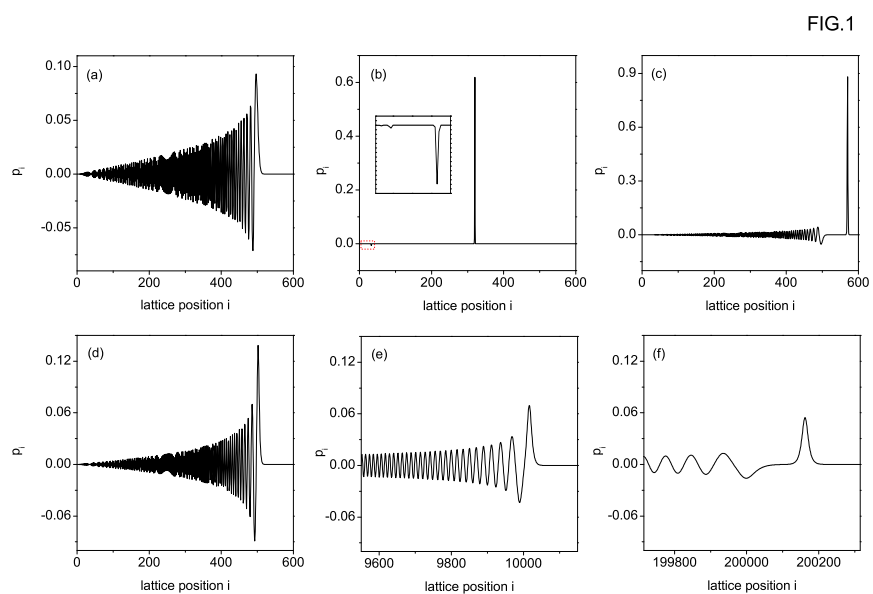
FIG. 6 The average energy scattering rates and the average rate of the energy "loss" at $E_a/E_b = 1/2$ on a semilogarithmic scale. (a), $\langle E'_a - E_a \rangle / E_a$ versus E_a . Inset is enlargement of rectangle. (b), $\langle E'_b - E_b \rangle / E_b$ versus E_b . (c), $\langle \Delta E \rangle / (E_a + E_b)$ versus $E_a + E_b$. The dot and star represent the results of solitary waves in the FPU lattice and in the pure anharmonic lattice, respectively.

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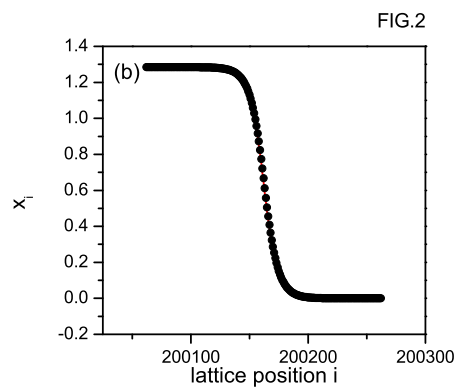
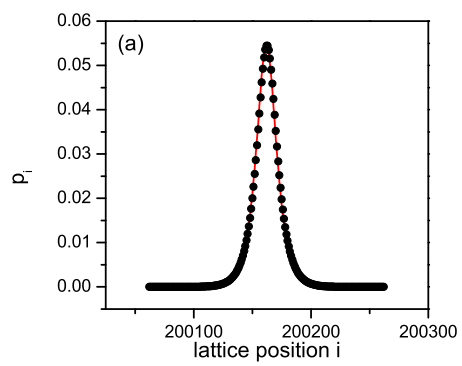


FIG.2

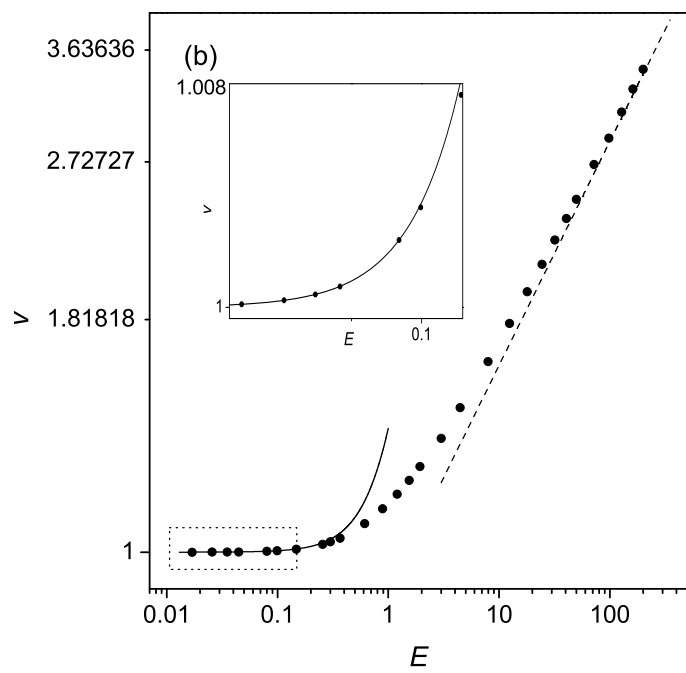
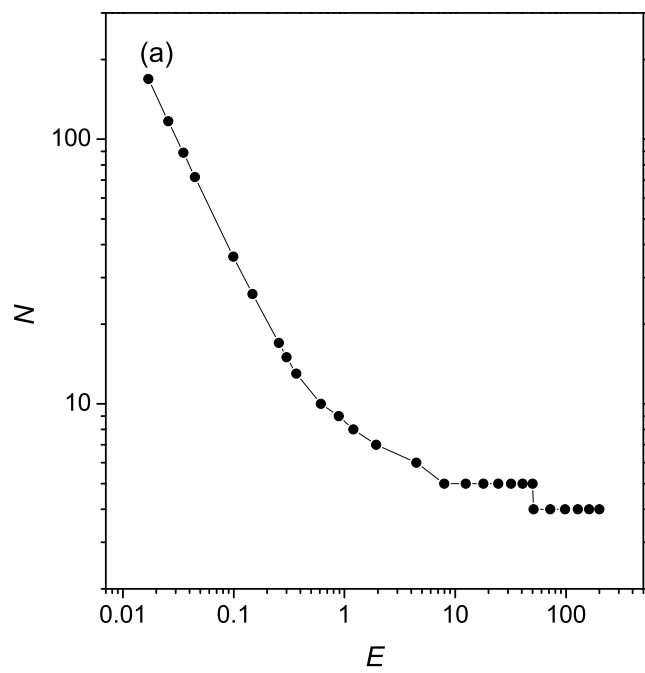


FIG.3

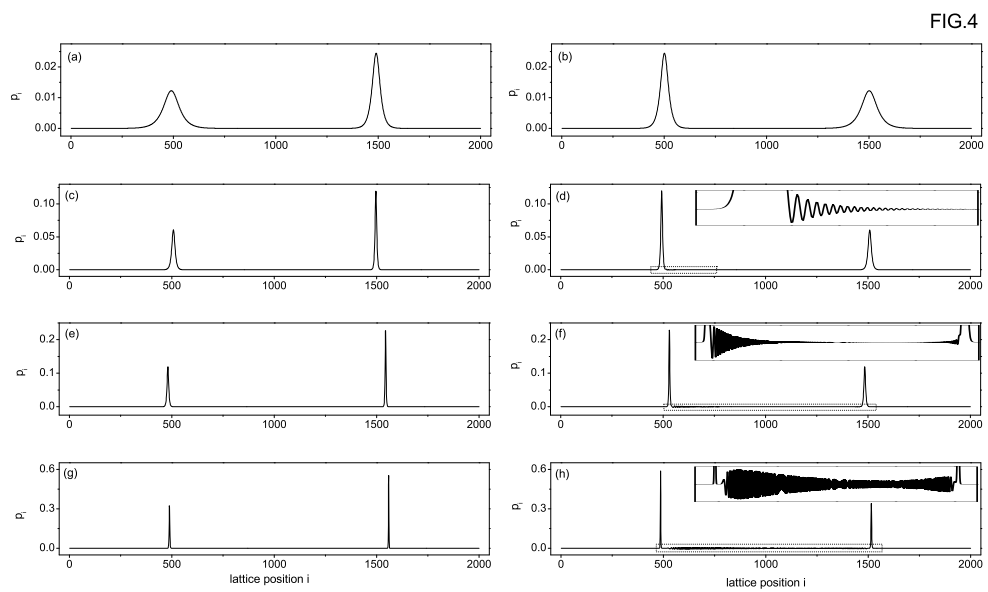


FIG.5

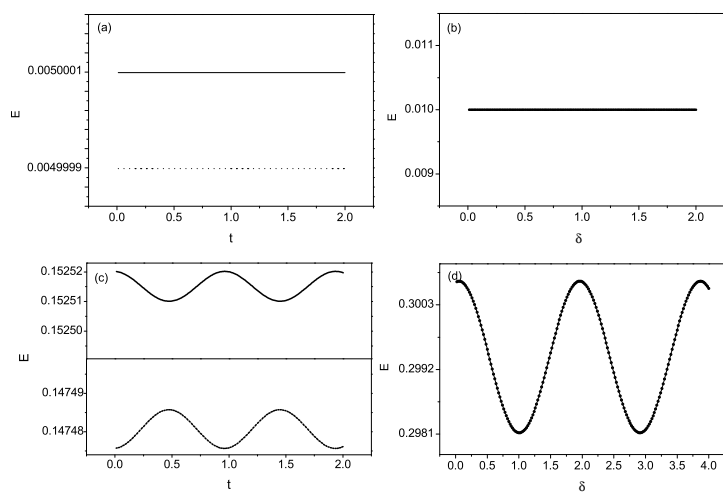


FIG.6

